

2,3,4,9-tetrahydro-1h-carbazol-3-ylacetonitrile  
40496-58-0 | DTXSID60300275

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 21.8

Global applicability domain: Inside

Local applicability domain index: 4.45e-01

Confidence level: 5.12e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Molinate</div> <div>Measured: 25.7</div> <div>Predicted: 14.8</div>	<div>Image not found</div> <div>2-(Thiocyanomethylthio)benzothiazole</div> <div>Measured: 209</div> <div>Predicted: 13.0</div>	<div>Image not found</div> <div>N,N-Diethylaniline</div> <div>Measured: 102</div> <div>Predicted: 12.8</div>
<div>Image not found</div> <div>4-Isobutylmorpholine</div> <div>Measured: 1.78</div> <div>Predicted: 2.69</div>		